3-Deoxy-manno-oct-2-ulopyranosonic acid
10149-14-1 | DTXSID80143949

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.24

Global applicability domain: Outside

Local applicability domain index: 1.68e-01

Confidence level: 8.71e-01

Nearest Neighbors from the Training Set

Image not found
7-Amino-4-hydroxynaphthalene-2-sulfonic acid
Measured: 2.40
Predicted: 4.77

Image not found
6-Amino-4-hydroxynaphthalene-2-sulfonic acid
Measured: 4.07
Predicted: 4.77

Image not found
2-Amino-5-methylbenzenesulfonic acid
Measured: 3.98
Predicted: 6.29

Image not found
Tris(2-hydroxyethyl) isocyanurate
Measured: 1.58
Predicted: 1.61

Image not found
4-Amino-1-naphthalenesulfonic acid sodium salt
Measured: 6.03
Predicted: 5.38